KNJ-235-A METHOD FOR LEVELING RESPONSE CHARACTERISTICS OF SPECTROSCOPE

DESCRIPTION

Technical Field

[0001] The present invention relates to a method for leveling a spectroscope response characteristic for correcting the difference between spectroscope response characteristics generated due to the difference between response characteristics of a light source, spectrograph, and sensor.

Background Art

[0002] To control measurement errors and fluctuations of a plurality of inspection instruments for mass production of products, it is frequently performed to adjust each inspection instrument by using an exclusive jig. However, in the case of calibration of the inspection instrument, lots of work times and predetermined man-hours are required when many check points are present and finally, the adjustment cost greatly influences a product price. Therefore, it is preferable to minimize the number of check points requiring adjustment. However, in the case of a product for which accuracy is requested, artifice is necessary.

[0003] For example, Patent Document 1 describes the following expression as a relative relational expression for showing the correlation between the measured value and the true value of a reproduced signal in order to reproduce an optical disk to be inspected by an optical-disk inspection instrument.

True value Y_i =Gain correction coefficient a_j ×measured value X_i +offset correction coefficient b_i (a)

X_i: Measured value of reproduced signal

Y_i: True value of reproduced signal

ai: Gain correction coefficient for correcting gain for each interval

b_i: Offset correction coefficient for correcting offset for each interval

Moreover, the gain correction coefficient a_j and the offset coefficient b_j are obtained for each interval. Furthermore, a method for calibrating measurement means in accordance with a calibrated value obtained by using the computing means and inspecting an optical disk to be inspected is described in Patent Document 1.

Patent Document 1: Japanese Patent Application Publication No. 2003-1897440

Disclosure of the Invention

[0004] However, when an object to be inspected has a frequency (wavelength) characteristic more complex than that of an optical disk and the reflection spectrum of an apple is measured in a wavelength range of 700 to 1,100 nm by using, for example, a discrete-type near infrared apparatus, there is a problem that individual difference between objects to be measured is large, which is not present in an optical disk.

Though the approximate expression (a) shown in Patent Document 1 is used, it is impossible to find a proper linear correction parameter as shown by linear correction data in Table 1.

Also when using the following approximate expression (b) using a more-complex polynomial,

$$y = k_0 + k_1 s + k_2 x^2$$
 (b)

it is impossible to find a proper polynomial parameter as shown by the polynomial correction data in Table 1.

[0005] [Table 1]

Adjustment line condition	Calibration method				
	MLR		PLS		
	SEP	Bias	SEP	Bias	
No adjustment	0.34	-0.42	0.35	-0.53	
700-1,100 nm linear correction	0.34	-1.07	0.32	-1.31	

700-1,100 nm polynomial correction	0.34	-0.48	0.31	-1.14
850-1,050 nm linear correction	0.34	-0.46	0.32	-1.24
850-1,050 nm polynomial correction	0.34	0.25	0.31	-1.06

(Note 1) Analysis algorithm

MLR (Multiple Linear Regression)

PLS (Partial Least Squares)

(Note 2)

SEP: Residual-error standard error (Standard error of bias-corrected expected value)

Bias: Average of differences between estimated values and chemical analysis values according to near infrared spectroscopy

[0006] Moreover, when moving a calibration model (hereafter referred to as model) for performing quantitative analysis and qualitative analysis by using the near infrared spectroscopy from a unit developing the model to another similar unit, an error occurs due to the difference between spectral-apparatus response characteristics. In the case of the quantitative analysis, there is a method referred to as bias correction method of the model as a correction method. However, this method is correction of an estimated result, which requires correction for each model and labor and whose operation is complicated.

However, the correction method for qualitative analysis is not developed yet.

[0007] It is an object of the present invention to provide a method for leveling response characteristics of a spectroscope for correcting the distortion of a spectrum generated due to the difference between spectroscope response characteristics so that a model developed by a parent unit can be used by a child unit.

To achieve the above object, a method of the present invention for leveling the response characteristic of a spectroscope provides a method for adjusting the response characteristic of a child unit to the response characteristic of a parent unit by subtracting the spectrum of a standard substance measured by the parent unit, for example, secondary-differential spectrum from the spectrum of the standard substance measured by the child unit, for example,

secondary-differential spectrum thereby obtaining the difference spectrum between the child unit and the parent unit, and thereby subtracting the difference spectrum from the secondary-differential spectrum of each sample to be measured by the child unit. By using the secondary-differential spectrum, there is an advantage that the shift of the base line is eliminated. [0008] As the spectrum of the standard substance, the spectrum of a sample to be measured, secondary-differential spectrum, or average spectrum of the spectrum of the sample and the secondary-differential spectrum is considered. In the case of the average spectrum, the following two cases are assumed: a case of measuring a plurality of spectrums by one sample to be measured and obtaining the average spectrum and a case of measuring a plurality of spectrums by a plurality of samples and obtaining the average spectrum.

[0009] An apparatus to which near infrared spectroscopy is applied is constituted of beam of light, spectrograph, and sensor. Wavelength characteristics, luminances, and sensitivities of them are delicately different for each individual piece and the spectroscope response characteristic which is the overall characteristic of the apparatus is delicately different for each apparatus. Moreover, a shift of the wavelength of a spectroscope occurs. However, the spectroscope response characteristic is peculiar to each apparatus when a light source, spectrograph, and sensor are decided.

[0010] Therefore, because a shift of absorbance value of a child unit in each wavelength from a parent unit similarly occurs in each sample to be measured, it is possible to correct a spectrum distortion generated due to the difference between spectroscope response characteristics by subtracting the shift of the absorbance value in each wavelength from the spectrum of each sample, for example, secondary-differential spectrum.

[0011] According to the present invention, in the case of a fruit sugar content selector, it is easy to move a sugar-content analytical distillation developed by a reference selection line (parent unit) to a plurality of other selection lines (child unit), difference between lines is eliminated, and the reliability of the selector is improved. Moreover, there are advantages that

the selector is easily maintained and persons are released from the hard work at the job site for correcting the difference between lines.

Brief Description of the Drawings

[0012] Figure 1 is an illustration showing an example of an apple sugar content selector;

Figures 2(a) and 2(b) are illustrations showing secondary-differential spectrums measured by near infrared apparatuses A and B;

Figure 3 is an illustration showing an example of applying a model developed by the near infrared apparatus A to the spectrum of the near infrared apparatus B;

Figure 4 is an illustration showing a difference spectrum obtained by subtracting the secondary-differential spectrum of an apple measured by the near infrared apparatus A from that of an apple measured by the near infrared apparatus B;

Figure 5 is an illustration showing an example of applying a model developed by the near infrared apparatus A to the leveling spectrum of the near infrared apparatus B; and

Figure 6 is an illustration showing a difference spectrum obtained by subtracting the average spectrum of secondary-differential spectrums measured by a parent unit from the average spectrum of secondary-differential spectrums measured by a child unit and the average spectrum of the parent unit.

Best Mode for Carrying Out the Invention

[0013] Best mode for carrying out the invention is described below. Figure 1 is one of the embodiments of the present invention, which shows an example of an apple sugar-content selector. In the case of the selector, a tungsten lamp is used for the light source, a diffraction grating is used for the spectrograph, and a diode array detector is used for the sensor.

[0014] At the stage for preparing a model by the parent unit in Figure 1(1), a plurality of samples (apples) 1 to be measured are measured by the sensor 2 of the parent unit to obtain the

secondary-differential spectrum 3 of the parent unit. Then, chemical analysis values 4 of the

samples (apples) 1 are obtained. A model 5 is obtained by the chemometrics method such as the multiple regression analysis in accordance with the data for the above secondary-differential spectrum 3 and the above chemical component values 4.

[0015] At the stage for obtaining the difference between spectral characteristics of the parent unit and child unit in Figure 1(2), a plurality of samples (apples) 6 to be measured are measured by the sensor 2 of the parent unit to obtain the average spectrum of the secondary-differential spectrums of the parent unit. Then, the same samples (apples) 6 to be measured are measured by the sensor 8 of the child unit to obtain the average spectrum 9 of the secondary-differential spectrums of the child unit. Moreover, the difference spectrum 10 between secondary-differential values is obtained by subtracting the average spectrum 7 of the parent unit from the average spectrum 9 of the child unit.

At the stage for leveling the spectral characteristics of the child unit in Figure 1(3), each sample (apple) 11 to be measured is measured by the sensor 8 of the child unit and the secondary-differential spectrum 12 of the child unit is measured to obtain a leveled secondary-differential spectrum 13 obtained by subtracting the difference spectrum 10 from the secondary-differential spectrum 12. By applying the model 5 to the leveled secondary-differential spectrum 13, a purposed chemical component value 14 is obtained.

[0016] Figure 2 is near infrared secondary-differential spectrums of apples (product class: Fuji) measured by two discrete-type near infrared apparatuses (NIRS6500 made by NIR Systems) (referred to as near infrared apparatuses A and B). The near infrared apparatus uses a tungsten lamp as a light source, a diffraction grating as a spectrograph, and silicon detector as a sensor.

[0017] The model of the following expression is developed through multiple regression in accordance with the secondary-differential values and sugar contents (Brix values) of spectrums of 100 apples measured by the near infrared apparatus A.

$$C = 16.035 - 266.386D2A(906) + 1351.578D2A(870)$$

... (1)

In this case, C denotes a Brix value and D2A(906) and D2A(870) are secondary-differential values of spectrums at 906 nm and 870 nm, respectively.

[0018] Figure 3 shows results of applying the model of the above expression (1) to a spectrum measured by the near infrared apparatus B. In this case, it is found that a negative bias of -0.42° Brix is generated.

[0019] Figure 4 is a difference spectrum obtained by subtracting the average spectrum of the near infrared apparatus A from the average spectrum of secondary-differential spectrums of the above 100 apples measured by the near infrared apparatus B. Figure 4 shows the wavelength range of 860 to 910 nm to be used for the model. It is found that the secondary-differential value of the near infrared apparatus B is slightly larger than that of the near infrared apparatus A in the wavelength region. At 906 nm, the secondary-differential value is large by 0.0021515 and at 870 nm, the value is large by 0.0008103. Therefore, when assuming that the secondary-differential values at 906 nm and 870 nm of the near infrared apparatus B are D2A(906)_B and D2A(870)_B respectively, a corrected value is obtained from the following expression.

$$D2A(906) = D2A(906)_B - 0.0021515$$

 $D2A(870) = D2A(870)_B - 0.0008103$... (2)

By substituting the value of expression (2) for the model of expression (1), it is possible to apply the model developed by the near infrared apparatus A to the spectrum measured by the near infrared apparatus B.

[0020] Figure 5 shows results of correcting and recalculating the data shown in Figure 3 by the above described method. A bias becomes 0.05° Brix and occurrence of errors produced due to the difference between spectroscope response characteristics is almost cancelled. This improvement degree is clear as a result of comparing with calibration result data of linear correction and polynomial expression correction in Table 1.

[0021] Figure 6 shows a difference spectrum obtained by subtracting the average spectrum of secondary-differential spectrums measured by the parent unit from the average spectrum of secondary-differential spectrum measured by the child unit and the average spectrum of the parent unit in a wavelength region of 850 to 1,050 nm together. When assuming a difference spectrum as $\Delta A(\lambda)$ and a secondary-differential spectrum of a sample measured by the child unit as $S_B(\lambda)$, a leveled secondary-differential spectrum $S_C(\lambda)$ is shown by the following expression.

$$S_{C}(\lambda) = S_{B}(\lambda) - \Delta A(\lambda) \qquad ... (3)$$

In this case, λ denotes a wavelength (nm).

Industrial Applicability

[0022] It is possible to apply leveling of the spectroscope response characteristic by the present invention to a line for measuring the spectrum of fruit moved by, for example, a belt conveyer and selecting the fruit in accordance with a chemical component value such as an obtained sugar content.